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A Family of Four-Step Exponential Fitted Methods for the Numerical Integration of the Radial Schrödinger Equation

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Abstract—A family of exponential four-step methods is developed for the numerical integration of the one-dimensional Schrödinger equation. The formula developed contains certain free parameters which allows it to be fitted automatically to exponential functions. The new methods integrate more exponential functions, and are very simple compared with the well-known sixth algebraic order Runge-Kutta type methods. Numerical results indicate that the new methods are much more accurate than other exponentially fitted methods.

Keywords—Schrödinger equation, Four-step methods, Exponential fitted methods, Resonance problem.

1. INTRODUCTION

In recent years, the radial Schrödinger equation has been the subject of great activity, the aim being to achieve a fast and reliable algorithm that generates a numerical solution.

The radial Schrödinger equation belongs to the problems of the form

$$y'' = f(x, y(x)). \tag{1}$$

The one-dimensional Schrödinger equation has the form:

$$y''(x) = \left[\frac{l(l+1)}{x^2} + V(x) - k^2\right] y(x), \tag{2}$$

where one boundary condition is $y(0) = 0$, with the other boundary condition being specified at $x = \infty$. Equations of this type occur very frequently in theoretical physics, for example [1], and there is a real need to be able to solve them both efficiently and reliably by numerical methods. In (2), the function $W(x) = l(l+1)/x^2 + V(x)$ is called *the effective potential*, for which $W(x) \to 0$ as $x \to \infty$, and k^2 is a positive real number denoting *the energy*. The boundary conditions are:

$$y(0) = 0, \tag{3}$$

and a second boundary condition, for large values of x, is determined by physical considerations.

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Boundary value methods based on either collocation or finite differences are not very popular for the solution of (2) due to the fact that the problem is posed on an infinite interval. Initial value methods, such as shooting, need to take into account the fact that $|y'(x)|$ is very large near $x = 0$. So, it is very inappropriate to use standard library packages for the numerical solution of (2).

One of the most popular methods for the solution of (2) is the **Numerov method.** This method is only of order four, but in practice, it has been found to have a superior performance to higher order four-step methods described in [2]. The reason for this, as was proved in [3], is that the Numerov method has the same phase-lag order as the four-step methods but it has a larger interval of periodicity. So, the investigation of linear multistep methods, with constant coefficients, is not a fruitful way to derive efficient high order methods.

An alternative approach to deriving higher order methods for (2) was given by Cash and Raptis [4]. In [4], a sixth order Runge-Kutta type method with a large interval of periodicity was derived. This method has a phase-lag of order six (while the Numerov method has phase-lag of order four) and an interval of periodicity much larger than the method of Numerov.

An alternative approach for developing efficient methods for the solution of (2) is to use exponential fitting. This approach is appropriate because for large x and $k^2 > 0$ the solution of (2) is *periodic.* Raptis and Allison [5] have derived a Numerov type exponentially fitted method. Numerical results presented in [5] indicate that these fitted methods are much more efficient than Numerov's method for the solution of (2). Since the work of Raptis and Allison [5], the idea of exponential fitting has been investigated by many authors. Perhaps the most significant work in this general area was that of Ixaru and Rizea [6]. They showed that, for the resonance problem defined by (2), it is generally more efficient to derive methods which exactly integrate functions of the form:

$$\left\{1, x, x^2, \dots, x^p, \exp\left(\pm vx\right), x\exp\left(\pm vx\right), \dots, x^m\exp\left(\pm vx\right)\right\} \tag{4}$$

than to use classical exponential fitting methods. A powerful low order method of this type was developed by Raptis [7]. Also Simos [8] has derived a four-step method of this type which gives much more accurate results compared with other four-step methods. Simos [9] has derived a family of four-step methods which gives more efficient results than other four-step methods. Also Raptis and Cash [10] have derived an exponential fitted method and Cash, Raptis, and Simos [11] have derived a method fitted to (4) with $m = 1$ and $p = 3$.

The purpose of this paper is to derive a family of four-step methods fitted to (4) and in particular to derive methods with $m = 0$ and $p = 7, m = 1$ and $p = 5$, and $m = 2$ and $p = 3$. The new methods are very simple compared with the well-known Runge-Kutta type methods. Also they have comparable accuracy and are much more accurate when compared with the exponentially fitted four-step methods proposed by Raptis [12,13] and Simos [8,9]. We have applied the new methods in *the resonance* problem for the one-dimensional radial Schrödinger equation.

2. EXPONENTIAL MULTISTEP METHODS

To solve, numerically, the initial value problem

$$y^{(r)} = f(x,y), \quad y^{(j)}(A) = 0, \qquad j = 0, 1, \dots, r-1, \tag{5}$$

ones uses the multistep methods of the form

$$\sum_{i=0}^{k} a_i y_{n+i} = h^r \sum_{i=0}^{k} b_i f(x_{n+i}, y_{n+i}) \tag{6}$$

over the equally spaced $\left\{x_i\right\}_{i=0}^{k}$ in $[A, B]$.

We may associate the method (6) with the operator

$$L(x)=\sum_{i=0}^{k}\left[a_i z\left(x+ih\right)-h^r b_i z^{(r)}\left(x+ih\right)\right], \tag{7}$$

where z is a continuously differentiable function.

DEFINITION 1. *The multistep method (6) is algebraic, respectively, exponential of order p if the associated linear operator L vanishes for any linear combination of the linearly independent functions $1, x, x^2, \dots, x^{p+r-1}$, respectively, $\exp(v_0 x), \exp(v_1 x), \dots, \exp(v_{p+r-1}x)$, where v_i, $i = 0, 1, \dots, p+r-1$ are real or complex numbers.*

REMARK 1. (See [3,14].) If $v_i = v$, for $i = 0, 1, \dots, n$, $n \le p+r-1$, then the operator L vanishes for any linear combination of

$$\exp(vx), x\exp(vx), x^2\exp(vx), \dots, x^n\exp(vx), \exp(v_{n+1}x), \dots, \exp(v_{p+r-1}x).$$

REMARK 2. (See [3,14].) Every exponential multistep method corresponds in a unique way to an algebraic multistep method (by setting $v_i = 0$, for all i).

LEMMA 1. *(For proof see [2,14].) Consider an operator L of the form (7). With $v \in \mathcal{C}$, $h \in \mathcal{R}$, $n \ge r$ if $v = 0$, and $n \ge 1$ otherwise, then we have*

$$L\left[x^m\exp(vx)\right]=0, \qquad m=0,1,\dots,n-1, \qquad L\left[x^n\exp(vx)\right]\neq 0, \tag{8}$$

if and only if the function φ has a zero of exact multiplicity s at $\exp(vh)$, where $s = n$ if $v \ne 0$, and $s = n - r$ if $v = 0$, $\varphi(w) = \rho(w)/\log^r w - \sigma(w)$, $\rho(w) = \sum_{i=0}^{k} a_i w^i$ and $\sigma(w) = \sum_{i=0}^{k} b_i w^i$.

PROPOSITION 1. *(For proof, see [3].) Consider an operator L with*

$$L\left[\exp\left(\pm v_i x\right)\right]=0, \qquad j=0,1,\dots,k\le\frac{p+r-1}{2}, \tag{9}$$

then for given a_i and p with $a_i = (-1)^r a_{k-i}$, there is a unique set of b_i, such that $b_i = b_{k-i}$.

In the present paper, we investigate the case $r = 2$.

3. THE NEW FAMILY OF METHODS

Consider the family of methods:

$$\begin{aligned}\bar{y}_n &= y_n - ah^2\left(y''_{n+2}-4y''_{n+1}+6y''_n-4y''_{n-1}+y''_{n-2}\right)\; y_{n+2}-2y_{n+1}+2y_n-2y_{n-1}+y_{n-2}\\ &= h^2\left(b_0y''_{n+2}+b_1y''_{n+1}+b_2\bar{y}''_n+b_1y''_{n-1}+b_0y''_{n-2}\right),\end{aligned} \tag{10}$$

where, for example, $y''_{n+2} = f(x_{n+2}, y_{n+2})$ with $x_{n+2} = x_n + 2h$.

The local truncation error (LTE) for this method in the classical case ($b_0 = 3/40, b_1 = 13/15, b_2 = 7/60$) is given by

$$\mathrm{LTE}=-\frac{h^8\left(3528\,ay_n^{(6)}+95\,y_n^{(8)}\right)}{30240}+O\left(h^{10}\right). \tag{11}$$

We denote as the 'classical case' the purely algebraic case with no exponential terms.

We require that the family of methods (10) should be exact for any linear combination of the functions:

$$\begin{aligned}&\text{Case I:} && \left\{1,x,x^2,x^3,x^4,x^5,x^6,x^7,\exp(\pm vx)\right\},\\ &\text{Case II:} && \left\{1,x,x^2,x^3,x^4,x^5,\exp(\pm vx),x\exp(\pm vx)\right\},\\ &\text{Case III:} && \left\{1,x,x^2,x^3,\exp(\pm vx),x\exp(\pm vx),x^2\exp(\pm vx)\right\}.\end{aligned} \tag{12}$$

To construct a method of the form (10) which must be exact for the functions (12), we require that the method (10) should be exact for:

$$\{1, x, \exp(\pm v_0 x), \exp(\pm v_1 x), \exp(\pm v_2 x), \exp(\pm v_3 x)\} \tag{13}$$

and then put:

$$\begin{aligned} &\text{Case I:} && v_0 = v_1 = v_2 = 0 \quad \text{and} \quad v_3 = v,\\ &\text{Case II:} && v_0 = v_1 = 0 \quad \text{and} \quad v_2 = v_3 = v,\\ &\text{Case III:} && v_0 = 0 \quad \text{and} \quad v_1 = v_2 = v_3 = v. \end{aligned} \tag{14}$$

The method (10) is exact for the functions $1, x$. Demanding that (10) should be exact for (13), we obtain the following system of equations for b_0, b_1, b_2 and a:

$$\begin{aligned} 2w_j^2 b_0 \cosh(2w_j) + 2w_j^2 b_1 \cosh(w_j) + b_2 w_j^2 - 2ab_2 w_j^4 [\cosh(2w_j) - 4\cosh(w_j) + 3] \\ = 2[\cosh(2w_j) - 2\cosh(w_j) + 1], \end{aligned} \tag{15}$$

where $w_j = v_j h$, $j = 0, 1, 2, 3$.

Solving for b_0, b_1, b_2 and a we obtain:

CASE I. $v_0 = v_1 = v_2 = 0$ and $v_3 = v$.

$$\begin{aligned} b_0 &= \frac{3}{40}, \qquad b_1 = \frac{13}{15}, \qquad b_2 = \frac{7}{60},\\ a &= \frac{34560\left[3\left(40 - 3w^2\right)\cosh(2w) - 8\left(13w^2 + 30\right)\cosh(w) - 7w^2 + 120\right]}{-483840\, w^4 \left[\cosh(2w) - 4\cosh(w) + 3\right]}. \end{aligned} \tag{16}$$

The above formulae are subject to heavy cancellations for small values of $w = vh$. In this case, it is much more convenient to use the below-mentioned series expansions for the coefficient a of the method.

$$a = \frac{95}{3528} - \frac{83w^2}{105840} + \frac{w^4}{68992} + \frac{577w^6}{10807286400} - \frac{773w^8}{36614882304} + O\left(w^{10}\right). \tag{17}$$

CASE II. $v_0 = v_1 = 0$ and $v_2 = v_3 = v$.

$$\begin{aligned} b_0 = \frac{1}{D}\Bigg\{ & 384\, w^3 \left[-26\cosh(w) + 16\cosh(2w) - 6\cosh(3w) + \cosh(4w) + 15\right]\\ & + 192\, w^4 \left[5\sinh(w) - 4\sinh(2w) + \sinh(3w)\right]\\ & - 32\, w^5 \left[57\cosh(w) - 30\cosh(2w) + 7\cosh(3w) - 34\right]\\ & + 16\, w^6 \left[13\sinh(w) + 4\sinh(2w) - 7\sinh(3w)\right] \Bigg\},\\ b_1 = \frac{1}{D}\Bigg\{ & 1536\, w^3 \left[26\cosh(w) - 16\cosh(2w) + 6\cosh(3w) - \cosh(4w) - 15\right]\\ & - 768\, w^4 \left[5\sinh(w) - 4\sinh(2w) + \sinh(3w)\right]\\ & - 32\, w^5 \left[164\cosh(w) - 76\cosh(2w) + 28\cosh(3w) - 7\cosh(4w) - 109\right]\\ & - 64\, w^6 \left[13\sinh(w) + 4\sinh(2w) - 7\sinh(3w)\right] \Bigg\},\\ b_2 = \frac{1}{D}\Bigg\{ & - 2304\, w^3 \left[26\cosh(w) - 16\cosh(2w) + 6\cosh(3w) - \cosh(4w) - 15\right]\\ & + 1152\, w^4 \left[5\sinh(w) - 4\sinh(2w) + \sinh(3w)\right]\\ & - 64\, w^5 \left[115\cosh(w) - 62\cosh(2w) + 13\cosh(3w) + \cosh(4w) - 67\right]\\ & + 32\, w^6 \left[39\sinh(w) + 12\sinh(2w) - 21\sinh(3w)\right] \Bigg\}, \end{aligned} \tag{18}$$

$$a = \frac{1}{(D\, b_2)}\Big\{ 192w\,[15 - 26\cosh(w) + 16\cosh(2w) - 6\cosh(3w) + \cosh(4w)]$$
$$+ 192\,w^2\,[5\sinh(w) - 4\sinh(2w) + \sinh(3w)] \qquad \text{(18 continued)}$$
$$+ 16\,w^4\,[13\sinh(w) + 4\sinh(2w) - 7\sinh(3w)]\Big\},$$

where $D = -192\,w^5[56\cosh(w) - 28\cosh(2w) + 8\cosh(3w) - \cosh(4w) - 35]$.

The above formulae are subject to heavy cancellations for small values of $w = vh$. In this case it is much more convenient to use the below-mentioned series expansions for the coefficients of the method.

$$\begin{aligned}
b_0 &= \frac{3}{40} - \frac{83\,w^4}{907200} + \frac{w^6}{295680} + \frac{577\,w^8}{31135104000} + O\left(w^{10}\right),\\
b_1 &= \frac{13}{15} + \frac{83\,w^4}{226800} - \frac{w^6}{73920} - \frac{577\,w^8}{7783776000} + O\left(w^{10}\right),\\
b_2 &= \frac{7}{60} - \frac{83\,w^4}{151200} + \frac{w^6}{49280} + \frac{577\,w^8}{5189184000} + O\left(w^{10}\right),\\
a &= \frac{95}{3528} - \frac{83\,w^2}{52920} + \frac{46601\,w^4}{273829248} - \frac{6328291\,w^6}{533967033600} + \frac{59172647\,w^8}{62794523151360} + O\left(w^{10}\right).
\end{aligned} \tag{19}$$

CASE III. $v_0 = v_1 = v_2 = v_3 = v$.

$$\begin{aligned}
b_0 = \frac{1}{D}\Big\{ & 64\,w^3\,[98\cosh(w) - 64\cosh(2w) + 29\cosh(3w) - 8\cosh(4w) + \cosh(5w) - 56]\\
& - 16\,w^4\,[56\sinh(w) - 50\sinh(2w) + 15\sinh(3w) + \sinh(4w) - \sinh(5w)]\\
& + 16\,w^5\,[100\cosh(w) - 32\cosh(2w) - 3\cosh(3w) + 5\cosh(4w) - \cosh(5w) - 69]\\
& - 16\,w^6\,[5\sinh(w) - 4\sinh(2w) + \sinh(3w)]\\
& + 16\,w^7\,[11\cosh(w) + 4\cosh(2w) - 3\cosh(3w) - 12]\\
& + 16\,w^8\,[3\sinh(w) - \sinh(3w)]\Big\},
\end{aligned}$$

$$\begin{aligned}
b_1 = \frac{1}{D}\Big\{ & - 64\,w^3\,[20\cosh(w) - \cosh(2w) - 14\cosh(3w) + 14\cosh(4w) - 6\cosh(5w) + \cosh(6w) - 14]\\
& + 16\,w^4\,[14\sinh(w) + 40\sinh(2w) - 75\sinh(3w) + 44\sinh(4w) - 9\sinh(5w)]\\
& - 16\,w^5\,[274\cosh(w) - 80\cosh(2w) - 15\cosh(3w) + 16\cosh(4w) - 3\cosh(5w) - 192]\\
& - 32\,w^6\,[4\sinh(w) - 6\sinh(2w) + 4\sinh(3w) - \sinh(4w)]\\
& + 64\,w^7\,[8\cosh(w) - 6\cosh(2w) + \cosh(4w) - 3] - 64\,w^8\,[3\sinh(w) - \sinh(3w)]\Big\},
\end{aligned}$$

$$\begin{aligned}
b_2 = \frac{1}{D}\Big\{ & - 128\,w^3\,[78\cosh(w) - 63\cosh(2w) + 43\cosh(3w) - 22\cosh(4w)\\
& \qquad + 7\cosh(5w) - \cosh(6w) - 42]\\
& + 32\,w^4\,[42\sinh(w) - 90\sinh(2w) + 90\sinh(3w) - 43\sinh(4w) + 8\sinh(5w)]\\
& + 32\,w^5\,[174\cosh(w) - 48\cosh(2w) - 12\cosh(3w) + 11\cosh(4w) - 2\cosh(5w) - 123]\\
& - 16\,w^6\,[16\sinh(w) - 16\sinh(2w) + 9\sinh(3w) - 4\sinh(4w) + \sinh(5w)]\\
& + 16\,w^7\,[40\cosh(w) - 8\cosh(2w) + 9\cosh(3w) - 4\cosh(4w) - \cosh(5w) - 36]\\
& + 96\,w^8\,[3\sinh(w) - \sinh(3w)]\Big\},
\end{aligned} \tag{20}$$

$$a = \frac{1}{(D\, b_2)} \Bigg\{ 24\, w^2 \left[14 \sinh(w) - 20 \sinh(2w) + 15 \sinh(3w) - 6 \sinh(4w) + \sinh(5w)\right]$$
$$+ 8w^3 \left[74 \cosh(w) - 16 \cosh(2w) - 9 \cosh(3w) + 6 \cosh(4w) - \cosh(5w) - 54\right]$$
$$+ 16\, w^6 \left[3 \sinh(w) - \sinh(3w)\right] \Bigg\}, \qquad \text{(20 continued)}$$

where

$$\begin{aligned} D = &-8w^6 \left[42 \sinh(w) - 48 \sinh(2w) + 27 \sinh(3w) - 8 \sinh(4w) + \sinh(5w)\right] \\ &+ 8w^7 \left[126 \cosh(w) - 48 \cosh(2w) + 3 \cosh(3w) + 4 \cosh(4w) - \cosh(5w) - 84\right]. \end{aligned}$$

The above formulae are subject to heavy cancellations for small values of $w = vh$. In this case, it is much more convenient to use the below-mentioned series expansions for the coefficients of the method:

$$\begin{aligned} b_0 &= \frac{3}{40} - \frac{83\, w^4}{302400} + \frac{2533\, w^6}{119750400} - \frac{4111\, w^8}{12454041600} + O\left(w^{10}\right), \\ b_1 &= \frac{13}{15} + \frac{83\, w^4}{75600} + \frac{103\, w^6}{14968800} - \frac{2921\, w^8}{778377600} + O\left(w^{10}\right), \\ b_2 &= \frac{7}{60} - \frac{83\, w^4}{50400} - \frac{373\, w^6}{6652800} + \frac{16949\, w^8}{2075673600} + O\left(w^{10}\right), \\ a &= \frac{95}{3528} - \frac{83\, w^2}{35280} + \frac{5329\, w^4}{11409552} - \frac{2198747\, w^6}{133491758400} + \frac{23467891\, w^8}{8721461548800} + O\left(w^{10}\right). \end{aligned} \tag{21}$$

4. STABILITY ANALYSIS

Consider the four-step method (10). We apply these methods to the test equation $y'' = s^2 y$. Setting $H = sh$, we obtain the stability polynomial

$$P(v) = A(H)v^4 + B(H)v^3 + C(H)v^2 + B(H)v + A(H), \tag{22}$$

where

$$\begin{aligned} A(H) &= 1 + H^2 b_0 + a b_2 H^4, \\ B(H) &= -2 + H^2 b_1 - 4 a b_2 H^4, \\ C(H) &= 2 + H^2 b_2 + 6 a b_2 H^4. \end{aligned} \tag{23}$$

Substituting in (22)

$$v = \frac{1+t}{1-t}, \tag{24}$$

we have

$$\begin{aligned} (1-t)^4 P(v) = &\left[2A(H) - 2B(H) + C(H)\right] t^4 + 2\left[6A(H) - C(H)\right] t^2 \\ &+ \left[2A(H) + 2B(H) + C(H)\right]. \end{aligned} \tag{25}$$

DEFINITION 2. *The method (10) is said to have an interval of periodicity* $\left(0, H_0^2\right)$ *if, for all* $H^2 \in \left(0, H_0^2\right)$, *the roots* v_i, $i = 1,2,3,4$ *of (22) satisfy*

$$v_1 = e^{i\theta(H)}, \quad v_2 = e^{-i\theta(H)}, \quad \text{and } |v_i| \le 1, \quad i = 3,4, \tag{26}$$

where $\theta(H)$ *is a real function of* H.

DEFINITION 3. *A method is said to be P-stable if it has an interval of periodicity is* $(0, \infty)$.

LEMMA 2. *All four-step methods with a stability polynomial given by (22) have interval of periodicity* $(0, H_0^2)$ *if*

$$P_1(H),\ P_2(H),\ P_3(H) \geq 0,$$
$$S(H) = P_2(H)^2 - 4P_1(H)P_3(H) \geq 0, \tag{27}$$

for all $H^2 \in (0, H_0^2)$, *where* $P_1(H) = 2A(H) - 2B(H) + C(H), P_2(H) = 12A(H) - 2C(H)$ *and* $P_3(H) = 2A(H) + 2B(H) + C(H)$.

PROOF. From (25) and (24) with $v = e^{i\theta}$, we obtain

$$t = i \tan\left(\frac{\theta}{2}\right), \quad \text{i.e., } t^2 \leq 0, \tag{28}$$

$$(1-t)^4 P(v) = P_1(H)\, t^4 + P_2(H)\, t^2 + P_3(H). \tag{29}$$

If $P_1(H) \neq 0$, (29) vanishes for

$$t^2 = \frac{-P_2(H) \pm \left[P_2(H)^2 - 4P_1(H)P_3(H)\right]^{1/2}}{2P_1(H)}, \tag{30}$$

and from (28), we obtain

(1) $P_2(H)^2 - 4P_1(H)P_3(H) \geq 0$, since from (28) we have that t^2 is a real number, and
(2) $P_1(H)P_2(H) \geq 0$ and $P_1(H)P_3(H) \geq 0$, since, based on (28), (30) ≤ 0.

So, assuming $P_3(H) \geq 0$, we have the conditions (27). ∎

Based on this theorem and substituting the values of a, b_0, b_1 and b_2 into (23), we have after straightforward calculations that:

Case I: $P_1(H)$, $P_2(H)$, $P_3(H)$, and $S(H) \geq 0$, for all $H^2 \in (0, 19.43328)$;
Case II: $P_1(H)$, $P_2(H)$, $P_3(H)$, and $S(H) \geq 0$, for all $H^2 \in (0, 19.43328)$;
Case III: $P_1(H)$, $P_2(H)$, $P_3(H)$, and $S(H) \geq 0$, for all $H^2 \in (0, \infty)$;

i.e., the method is P-stable.

For comparison purposes, we will calculate the interval of periodicity of the four-step methods produced by Simos [9] (Algorithms III, IV and Case II), which are the most accurate methods for the resonance problem of the Schrödinger equation (as it is shown in [9]).

Consider the method of [9]

$$y_{n+2} + a_0(y_{n+1} + y_{n-1}) + y_{n-2} = h^2\left[b_0\left(y''_{n+2} + y''_{n-2}\right) + b_1\left(y''_{n+1} + y''_{n-1}\right) + b_2 y''_n\right]. \tag{31}$$

For this method,

$$A(H) = 1 + H^2 b_0, \quad B(H) = -1 + H^2 b_1, \quad C(H) = H^2 b_2. \tag{32}$$

So, based on the above lemma, substituting a_0, b_0, b_1, b_2, we have:

Algorithm III of [9]: $P_1(H)$, $P_2(H)$, $P_3(H)$, and $S(H) \geq 0$, for all $H^2 \in (0, 13.46056)$;
Algorithm IV of [9]: $P_1(H)$, $P_2(H)$, $P_3(H)$, and $S(H) \geq 0$, for all $H^2 \in (0, 9.86944)$;
Case II of [9]: $P_1(H)$, $P_2(H)$, $P_3(H)$, and $S(H) \geq 0$, for all $H^2 \in (0, 9.86991)$.

5. NUMERICAL ILLUSTRATIONS

In this section, we present some numerical results to illustrate the performance of our method. We consider the numerical integration of the Schrödinger equation

$$y''(x) = (V(x) - k^2)y(x), \tag{33}$$

in the well-known case where the potential $V(x)$ is the Woods-Saxon potential

$$V(x) = \frac{u_0}{(1+z)} - \frac{u_0 z}{\left[c(1+z)^2\right]}, \tag{34}$$

with $z = \exp[(x - X_0)/a]$, $u_0 = -50$, $c = 0.6$ and $X_0 = 7.0$. In order to solve this problem numerically, we need to approximate the true (infinite) interval of integration $[0, \infty)$ by a finite interval. For the purpose of our numerical illustration, we take the domain of integration as $0 \le x \le 15$. We consider (33) in a rather large domain of energies, i.e., $[1, 1000]$. The problem we consider is the so-called *resonance problem.*

In the case of positive energies $E = k^2$, the potential dies away faster than the term $l(l+1)/x^2$; equation (2) effectively reduces to

$$y''(x) + \left(k^2 - \frac{l(l+1)}{x^2}\right) y(x) = 0, \tag{35}$$

for x greater than some value X.

The above equation has linearly independent solutions $kxj_l(kx)$ and $kxn_l(kx)$, where $j_l(kx)$, $n_l(kx)$ are the **spherical Bessel and Neumann functions**, respectively. Thus, the solution of equation (2) has the asymptotic form (when $x \to \infty$)

$$\begin{aligned} y(x) &\simeq Akxj_l(kx) - Bkxn_l(kx) \\ &\simeq AD\left[\sin\left(kx - \frac{\pi l}{2}\right) + \tan\delta_l \cos\left(kx - \frac{\pi l}{2}\right)\right], \end{aligned} \tag{36}$$

where δ_l is the **phase shift** which may be calculated from the formula

$$\tan\delta_l = \frac{y(x_2)S(x_1) - y(x_1)S(x_2)}{y(x_1)C(x_2) - y(x_2)C(x_1)}, \tag{37}$$

for x_1 and x_2 distinct points on the asymptotic region with $S(x) = kxj_l(kx)$ and $C(x) = kxn_l(kx)$.

Based on (36) and (37), we have that the normalization factor D is given by (see for details [3])

$$D \approx \frac{y(x_1)}{kx_1\left[\cos(\delta_l)S(x_1) + (-1)^l \sin(\delta_l)C(x_1)\right]}. \tag{38}$$

Since the problem is treated as an initial-value problem, one needs y_0, y_1, y_2 and y_3 before starting a four-step method. From the initial condition, $y_0 = 0$, it is easy to see that, for values of x close to the origin, the solution behaves as $y(x) = cx^{l+1}$ (see for details [3]). To calculate y_2 and y_3, we use the two-step exponentially fitted method of Raptis [7]. With these starting values, we evaluate at some point of the asymptotic region the phase shift δ_l and the normalization factor D from the above relations.

For positive energies one has the so-called resonance problem. This problem consists either of finding **the phase shift** δ or finding those k^2, for $k^2 \in [1, 1000]$, at which δ equals $\frac{\pi}{2}$ (see for details [1,15]).

The boundary conditions for this problem are:

$$\begin{aligned} y(0) &= 0, \\ y(x) &= \cos\left[\sqrt{E}\,x\right], \qquad \text{for large } x. \end{aligned}$$

The domain of numerical integration is $[0, 15]$. To calculate the phase shift δ using the relation given by (37), we use as $x_1 = 15$ and $x_2 = 15 - h$.

In our numerical illustration, we find the positive *eigenenergies or resonances* by the six methods:

Method M I:	Method derived by Simos (Method IV of [9]),
Method M II:	Method derived by Simos (Method V of [9]),
Method M III:	Method derived by Simos (Case II—Method VII of [9]),
Method M IV:	New exponential-fitted method (Case I of the family),
Method M V:	New exponential-fitted method (Case II of the family),
Method M VI:	New exponential-fitted method (Case III of the family).

The numerical results obtained for the seven methods were compared to the true solution to the Woods-Saxon potential resonance problem. This true solution was obtained correct to six decimal places using the analytical solution. Table 1 shows the absolute errors of the computed phase shifts for the eigenenergies given in the first column in 10^{-6} units (i.e., $\left|\delta_{\text{computed}} - \frac{\pi}{2}\right|$) for different choices of constant stepsize, which are shown in column 2. The empty cells indicate that the corresponding absolute errors are larger than the format allowed.

Table 1. Absolute errors, in 10^{-6} units, of the resonances calculated by the six algorithms M I–M VI.

The resonance	h	M I	M II	M III	M IV	M V	M VI
53.588872	1/16	104	52	29	12	1	0
	1/32	2	1	0	1	0	0
	1/64	0	0	0	0	0	0
163.215341	1/16	1125	360	197	92	6	0
	1/32	19	6	0	2	0	0
	1/64	0	0	0	0	0	0
341.495874	1/16	14424	1581	134	245	65	6
	1/32	141	26	9	6	1	1
	1/64	1	1	0	1	0	0
989.701916	1/16			612894	8765	123	9
	1/32	4080	152	80	18	7	2
	1/64	46	4	2	3	1	0

The performance of the different methods is dependent on the choice of the fitting parameter v. For the purpose of obtaining our numerical results, it is appropriate to choose v in the way suggested by Ixaru and Rizea [6]. That is, we choose

$$v = \begin{cases} \left(-50 - E\right)^{1/2}, & \text{for } x \in [0, 6.5], \\ \left(-E\right)^{1/2}, & \text{for } x \in (6.5, 15]. \end{cases}$$

For a discussion of the reasons for choosing the values 50 and 6.5 and the extent to which the results obtained depend on these values see [6, p. 25].

All computations were carried out on an IBM *PC*-AT 80386 with an 80387 mathcoprocessor of the Informatics Laboratory of Agricultural University of Athens using double precision arithmetic (16 significant digits accuracy).

6. CONCLUSION

We must note that the new methods are very simple (compared with the Runge-Kutta-type hybrid methods of Cash, Raptis and Simos (see [10,11]) and much more accurate compared with the methods proposed by Raptis [12,13] and Simos [9]. We note that the methods produced by Simos [9] are the most accurate four-step methods in the literature for the resonance problem of the radial Schrödinger equation as this has been proved by numerical results shown in [9].

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